

[Contact PI] [Compound code] [Date]	[Compound structure]	Instructions: This report card should provide data on a <u>single</u> compound--please do not include data from different compounds, even if they share the same scaffold. You may provide info on the activities of related compounds in the "comments" section. Please replace bracketed text with the content indicated. Italicized text indicates recommended units.
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Category	Parameter	Observed Activity	Target for Hit-to-Lead Chemistry	Target for Lead Optimization	Comments
Chemistry	cLogP				
	LogP				
	PSA				
	Molecular weight				
	Rotatable bonds				
	Number of chiral centers				
	H-bond donors				
	H-bond acceptors				
	Solubility (vehicle)	<i>mg/ml</i>			
	Scale-up feasibility	<i>Low/Med/High</i>			[Largest scale to date, # of steps, yield]
	Salt form				
	Crystallinity				
	SAR				[# of analogs tested, range of activity, commercially available analogs tested?]
	Patent protection	<i>Low/Med/High</i>			[Composition of matter, methods on candidate and back-ups. Note limitations]
Pharmacology	Activity in primary assay (potency)	<i>nM or μM</i>			
	Activity in secondary assay	<i>nM or μM</i>			
	Activity in tertiary assay	<i>nM or μM</i>			
	Selectivity (related family)	<i>fold</i>			
	Selectivity (unrelated family)	<i>fold</i>			
	Activity in broad screening panel				
	Clinically relevant biomarker available?	<i>Y/N</i>			
	Mechanism	<i>agonist/antagonist</i>			

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Pharmacokinetics/ Metabolism	Bioanalytical method available?	Y/N			
	T _{max}	<i>h</i>			[species, mg/kg, route of administration]
	T _{1/2}	<i>h</i>			[species, mg/kg, route of administration]
	C _{max}	<i>ng/ml</i>			[species, mg/kg, route of administration]
	AUC				[species, mg/kg, route of administration]
	Brain to Plasma	%			[species, mg/kg, route of administration]
	Bioavailability	%			[species, mg/kg, route of administration]
	V _{ss}	<i>L/kg</i>			[species, mg/kg, route of administration]
	CL	<i>L/kg/h</i>			[species, mg/kg, route of administration]
	Brain to Blood	%			
	in vitro permeability [indicate assay, e.g., PAMPA]				
	P-glycoprotein transport	<i>BAAB ratio</i>			
	Plasma Protein Binding	%			
	Microsomal Stability	<i>% remaining</i>			
	P450 Inhibition (CYP3A, 2C9 etc)	<i>IC50</i>			
	P450 Inhibition, time independent	<i>IC50 shift</i>			
	CYP induction	<i>% +ve control</i>			
	PK-PD relationship established?	Y/N			
Human dose and regimen estimate (where possible)	Y/N				
Toxicity and Safety	Cytotoxicity (cells)				
	Ames	Y/N			
	hERG	%			
	Preliminary rat CV				
	Preliminary rat pulmonary				
	Chromosome aberration				
	CNS effects (e.g., Irwin test)				
	Acute toxicity				[species]
	14-day toxicity				[species]